

Solutions for Innovation

JNM-ECZS series

NMR spectrometer Z



JEOL Ltd.

Easy, compact and high performance!

NMR spectrometer Z

JNM-ECZS series

The ECZS NMR spectrometer (JNM-ECZS series) has functionality and performance of the high-end ECZR series, yet in a compact, space saving design. Through the combination of advanced software with highly reliable hardware, all routine measurements can be automated.

Using high sensitivity auto tune probes, including the optional SuperCOOL probe which features cryogenically cooled technologies, JNM-ECZS affords the world's best-in-class sensitivity.

The high performance can be demonstrated in many application fields.



Major Features

Smallest spectrometer in the world*

The JNM-ECZS spectrometer incorporates the instrumental performance normally only found in high end research models. However, the main spectrometer chassis has a footprint of only 57% of comparable JNM-ECS instruments, thus making it the smallest NMR spectrometer operating at 400 MHz in the world. In combination with superconducting magnets (SCM) which feature ultra-small stray magnetic fields, a more flexible installation layout is possible.

*Compared to 400 MHz NMR spectrometers as of March 2015.

Advanced architecture using STS

The JNM-ECZS spectrometer is equipped with JEOL's newly-developed Smart Transceiver System (STS), which uses a fusion of the latest integrated digital circuit and high frequency technologies. By implementing the STS technology and the multi-sequencer which has been cultivated from earlier models, the standard 8 frequency sources are freely controllable regardless of whether they are synchronized or not. It cannot only execute all pulse programs used in routine work in a stress-free manner, but also execute very complex pulse programs with ease. Pulse sequence editing is also possible.

High stability and high accuracy digital spectrometer

The JNM-ECZS spectrometer provides fully digital control of RF generation, NMR lock and shim units, in order to maintain the high stability essential for high quality spectra. The excellent stability of the spectrometer can be demonstrated in its power of solvent suppression and difference spectra measurement, enabling the acquisition of many types of NMR spectra easily.

ROYALPROBE™

The ROYALPROBE™ has been designed based on the essence of JEOL's probe technologies and is the standard probe supplied with the spectrometer. It achieves a ^1H sensitivity approximately double that of existing auto tune direct detection probes. Users benefit from both the ease of use and a much reduced measurement time particularly in a modern NMR measurement facility which requires speed and performance. In addition, specialty probes such as cryogenic probes and triple-resonance probes are available as options. Please talk to your local JEOL specialist for your application.

ROYALPROBE™ HFX

The ROYALPROBE™ HFX is an unprecedented room-temperature probe that performs switching between double-resonance and triple-resonance modes. Purchasing a ROYALPROBE™ HFX in combination with high performance of the NMR spectrometer Z, makes it possible to record $^{13}\text{C}\{-^1\text{H}\}\{^{19}\text{F}\}$, $^1\text{H}\{-^{19}\text{F}\}$, etc. In the current NMR measurement sites, which require analysis of fluorinated compounds, this innovative ROYALPROBE™ HFX is an optimum probe.

Latest software and automation technology

The JNM-ECZS spectrometer uses the latest version of "Delta" software for both spectrometer control and for data processing. The excellent automation interface of Delta, together with gradient shimming applied as standard for each sample, ensures automatic measurements yield optimized resolution in a simple operation. When combined with an auto sample changer and auto tuning, all routine measurements can be automated.

Network spectrometer

The JNM-ECZS spectrometer is truly a networked device. The spectrometer can be operated separately from the operation terminal and can be controlled from any computer on the network.



Automation of all routine measurements

New auto tuning unit

In 1985, JEOL became a forerunner of an auto tuning unit. Since then, JEOL has been offering precise automatic tuning & matching system with stable operation, over the full multinuclear range. JEOL's new "Auto Tune Unit Z" has been developed for further ease of use based on our long experience of auto tuning technology. The availability of a reliable auto tuning mechanism is a prerequisite function for successful sequential automatic measurements including multinuclear measurements. The standard auto tune probe, which covers the frequency ranges of $^1\text{H}/^{19}\text{F}$ and ^{109}Ag to ^{31}P (thus includes almost all NMR nuclei), is designed to be used with this auto tune unit. This eliminates the need to manually tune the probe from underneath the SCM. The new "Auto Tune Unit Z" can be used with all NMR probes which JEOL is supporting. New auto tune probes operate almost noiselessly and tuning & matching information is memorized within each probe. The adoption of a single-touch quick coupler facilitates fast and easy coupling & decoupling the probe and Auto Tune Unit Z.

*For the ROYALPROBE™ HFX, an additional accessory is required.



Auto Tune Unit Z and head amplifier chassis

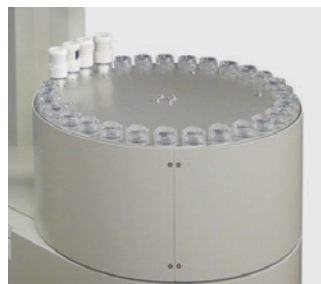


Adoption of a single-touch quick coupler made coupling and decoupling the probe from the Auto Tune Unit easy.

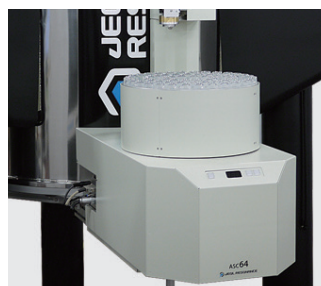
Auto sample changers

JEOL's Delta auto measurement function truly demonstrates its power and flexibility in sequential measurements at laboratories where very many samples are measured daily. JEOL's auto sample changers are designed to avoid direct contact with the sample tubes, so safe transfer of tubes of various tube diameters and shape is achieved. The JackBean series (models for 30, 64, and 100 tubes) transfer samples using a manipulator, while the ASC24 (24 tubes with exchangeable sample trays) is located on top of the SCM. On the compact JackBean series, samples are placed at low level so a step ladder is not needed to add or remove samples. For the JackBean series, "Pre-cool ASC30" that cools samples, has also been added.

JackBean series



ASC30 (30 sample positions model)



ASC64 (64 sample positions model)



ASC100 (100 sample positions model)



ASC24 (24 samples type)
The ASC24 sample changer is a carousel type and is located on top of the SCM, so no additional installation area is required. The exchangeable sample carousel allows advance preparation of multiple trays.



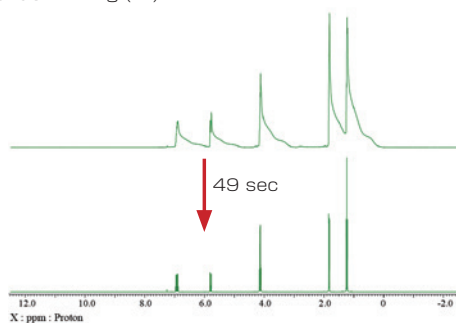
Pre-cool ASC30

The best-in-class resolution – always.

Gradient shimming measures the magnetic field distribution in the sample using magnetic field gradients and calculates the shim values necessary to correct the inhomogeneities. Correction of high order shims, which can require several hours even for a skilled engineer, can be optimized in a very short time. Even for volume limited solutions or samples in different solvents, gradient shimming takes place automatically, and so NMR spectra are obtained with optimum resolution. However, in the case of solvents with more than one signal such as methanol- d_4 and toluene- d_8 , the appropriate gradient shimming method using a shaped selective excitation pulse is selected automatically. Strong signals of ^1H or ^{19}F can also be used for gradient shimming, so that even for samples where a deuterated solvent is not used, optimization of resolution is still possible.

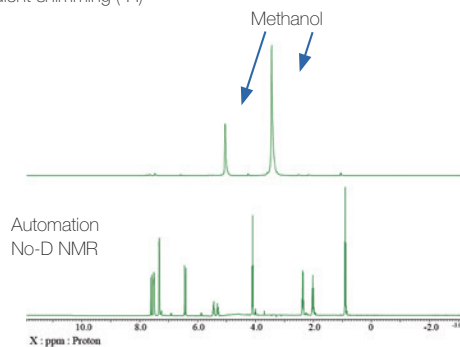
3D-gradient shimming, which was started to be installed in Delta V5.2, can automatically compensate for no-spin resolution. This feature allows for optimization of resolution in any states.

Gradient shimming (^2H)



Spectrum before and after resolution adjustment by gradient shimming. High resolution has been achieved in 49 sec.

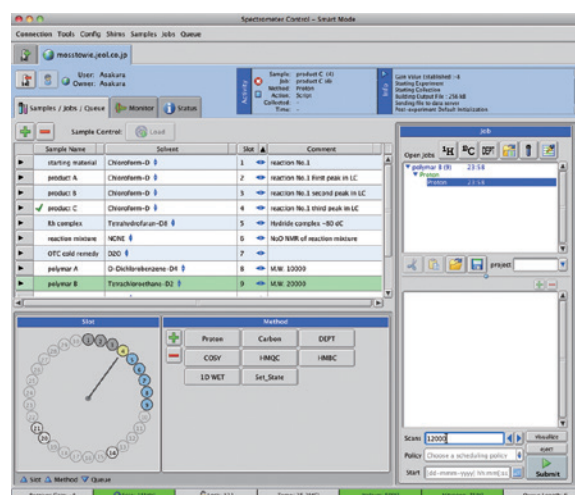
Gradient shimming (^1H)



No-D NMR measurement using resolution adjustment by selective gradient shimming for several signals solvent (top). Solvent signals are automatically suppressed by the 'WET' method (bottom).

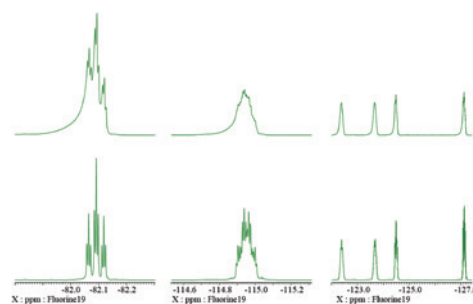
Competent Assistant

The JNM-ECZS spectrometer uses Delta to control the instrument and process data automatically. After sample setting, entering the sample name and solvent, Delta can handle everything: transferring the sample, probe tuning, resolution adjustment, measurement, data processing, and printing. The standard auto measurement function handles not only one dimensional measurements of ^1H & ^{13}C , but many other measurements including two dimensional NMR. These include options such as variable temperature, and performing experiments on several different nuclei sequentially. Experiment scheduling can be controlled easily, allowing for longer experiments to be run during nights or weekends. Data will be collected, processed, and stored, allowing for an entire day's worth of experiments to be queued up to run without further input.



Smart mode

Gradient shimming (^{19}F)



Resolution adjustment is possible by gradient shimming in the same manner as ^1H , by selecting the ^{19}F signal.

JEOL's ultra high sensitivity cryogenic probes realizing the best-in-class sensitivity

Astonishing high sensitivity "SuperCOOL probe"

JEOL's cryogenic probes are ultra high sensitivity probes with significantly improved performance achieved by cooling the detection coils. Two models of these probes are available; UltraCOOL probe and SuperCOOL probe. While the UltraCOOL probe offers the highest performance, the SuperCOOL probe offers greatly improved sensitivity but with lower price and reduced running cost. The SuperCOOL probe achieves sensitivity approaching three times that of conventional probes for ^{13}C thus reducing measurement time to one-ninth.

Open type SuperCOOL probes employ a cooling system using a liquid nitrogen tank. As open cooling does not require a refrigerator, it offers very low running costs. UltraCOOL probes and closed type SuperCOOL probes use a circulation cooling system. In addition to having greater cooling capability and thus giving higher sensitivity, circulation cooling removes the need to refill a cryogen dewar.

Either probe can control the sample temperature over a very wide range (-40°C to 150°C). Use of an optional probe lifter enables easy exchange of probes and can also be used with other probes.



SuperCOOL probe

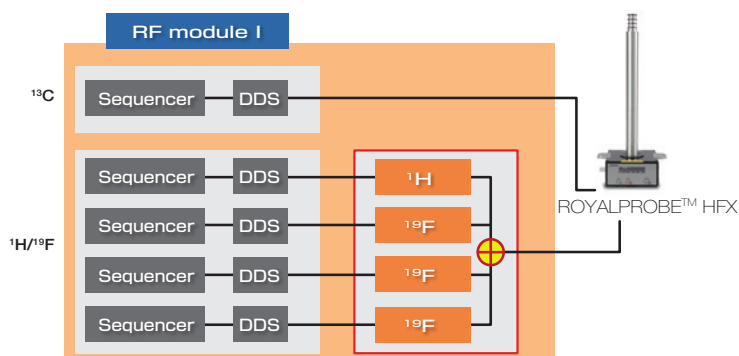


Probe Lifter

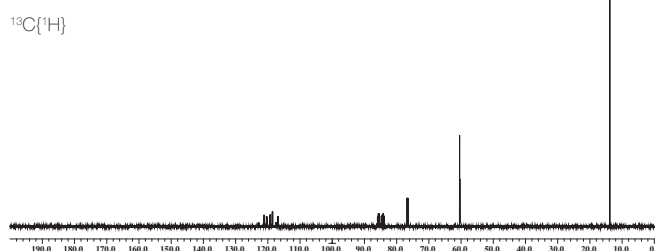
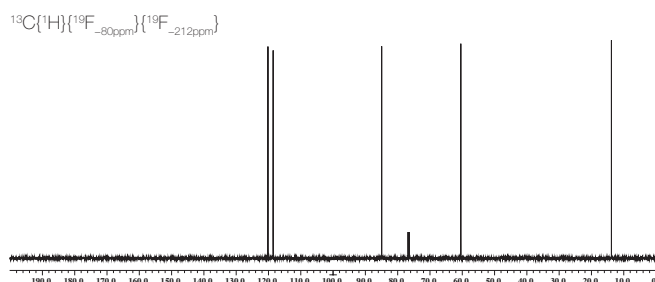


ROYALPROBE™ HFX

Example of configuration for ROYALPROBE™ HFX



Simultaneous output of ^1H and ^{19}F from the single high frequency source.



^{13}C spectrum of $\text{CF}_3\text{CH}(\text{F})\text{CF}_2\text{CH}_2\text{CH}_3$ measured on JNM-ECZ400S with ROYALPROBE™ HFX.

“ROYALPROBE™ HFX” performing triple resonance experiments with a 2 channel spectrometer

The ROYALPROBE™ HFX is an unprecedented room-temperature probe that performs switching between double resonance and triple resonance.

In the double resonance mode, this room-temperature probe can be used as an unprecedented ROYALPROBE™. In the case of analyzing fluorine-containing compounds that draw attention, the probe is used by switching to the triple resonance mode.

The triple resonance mode of the ROYALPROBE™ HFX allows simultaneous RF pulses on ^1H , ^{19}F and an X nucleus. Many important new materials, including pharmaceutical compounds, have ^1H and ^{19}F in their structure so simultaneous decoupling of ^1H and ^{19}F is essential, for example when measuring ^{13}C .

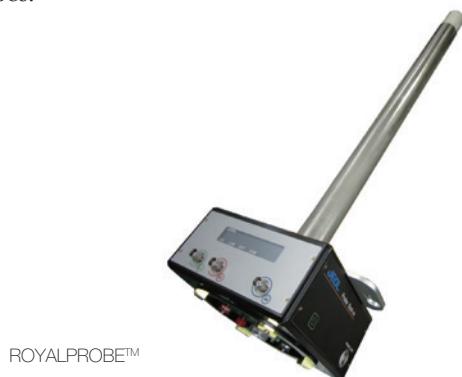
With a conventional NMR system, each of the three nuclei requires a separate frequency source (r.f. channel). However, JNM-ECZS requires just 2 r.f channels and enables triple resonance experiments using JEOL's unique multi-sequencer method. Experiments such as $^{13}\text{C}\{^1\text{H},^{19}\text{F}\}$ require only the addition of a ROYALPROBE™ HFX to the standard spectrometer.

* ROYALPROBE™ HFX: ROYALPROBE™ with triple-resonance $^1\text{H}/^{19}\text{F}/\text{X}$ capability.



High sensitivity probe ROYALPROBE™ as standard

The ROYALPROBE™, high-sensitivity solution state probe, is supplied as standard with the JNM-ECZS spectrometer. Using JEOL's latest probe technologies, it has double the ^1H sensitivity of conventional broadband probes, but without reducing ^{13}C sensitivity. Previously, two configurations of probes, direct probes and inverse probes have been used depending on the requirement. However, the high ^1H sensitivity of ROYALPROBE™ matches inverse probe performance. Thus JNM-ECZS offers improved detection limits and shorter measurement times by providing the performance of both types of probes without the need to exchange probes.



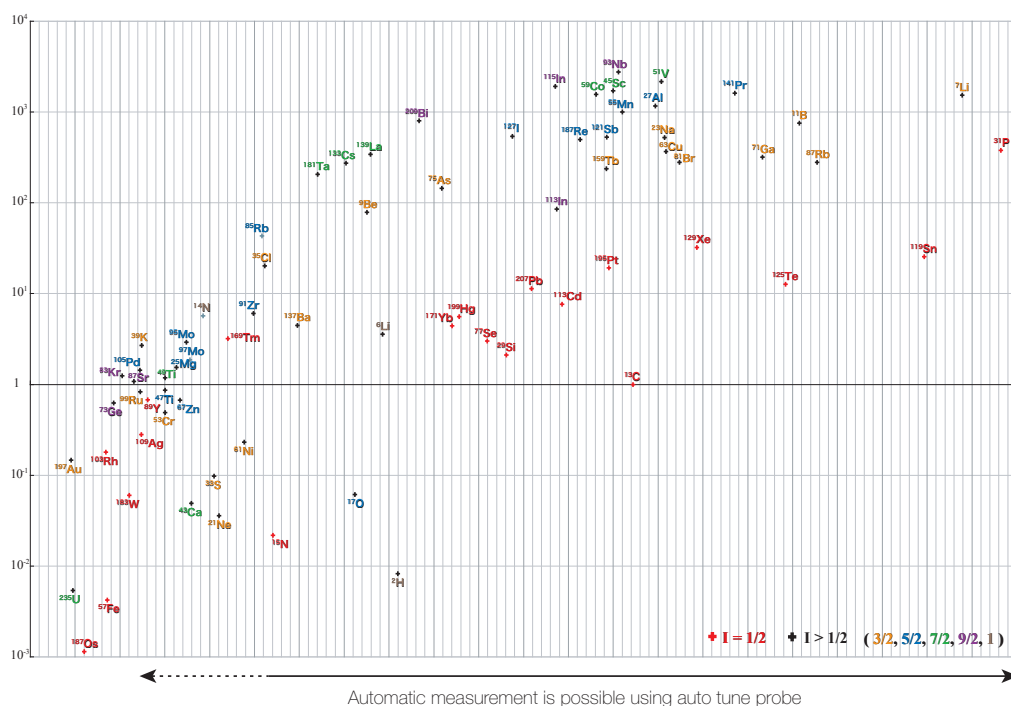
ROYALPROBE™

Wide range of probes available

The JNM-ECZS spectrometer can accommodate not only ROYALPROBE™, SuperCOOL probe, and ROYALPROBE™ HFX, but also more specialized probes such as high resolution 10 mm auto tune, 3 mm micro, low frequency probes, and ^{29}Si background free probe. Please talk to your local JEOL specialist for your application.



Resonance frequencies of NMR active nuclei and relative sensitivities.



Compatible with the latest applications

qNMR (quantitative NMR)

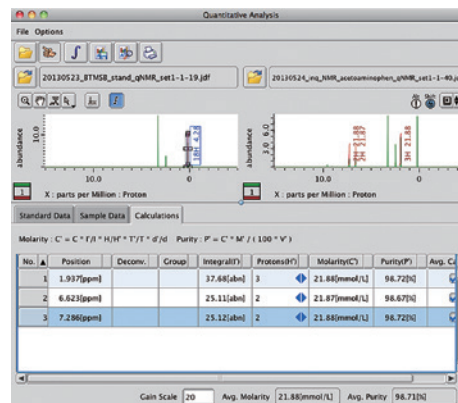
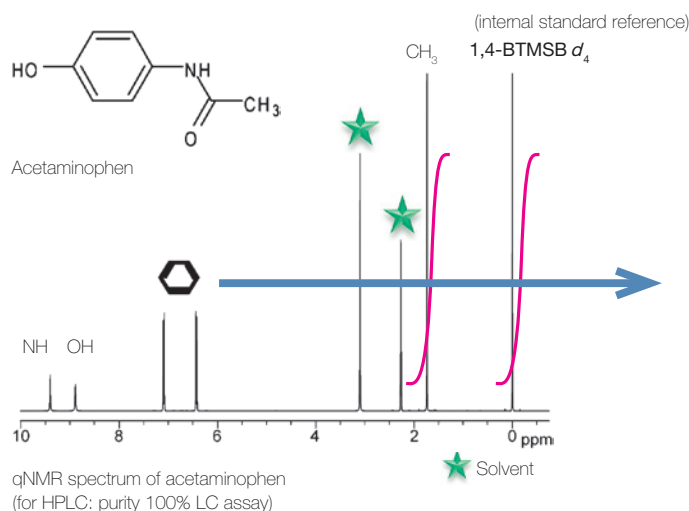
Quantitative analysis technology as specified by Pharmacopeia and official analytical methods

Application Example of AQARI*1

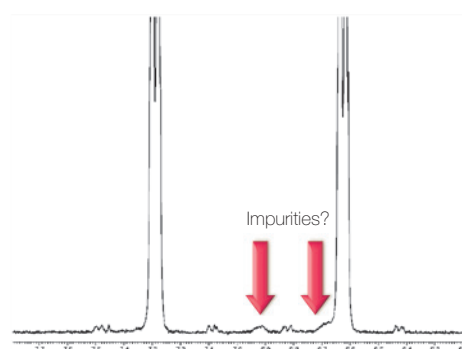
Purity analysis of acetaminophen

The purity analysis result of acetaminophen reagent using AQARI is shown below.

4-Bis(trimethylsilyl)benzene- d_4 *2 was used as the qNMR internal standard material and the ^1H signal from the CH_3 group of acetaminophen was used for the quantitation. After analysis and calculation according to formula (1), a purity value of 98.4% was obtained. So it is shown that AQARI can handle purity analysis and conformation of impurities simultaneously. As it enables acquisition of information such as degradation over a period of time, it can be used in quality control.



qNMR function of Delta software



Expansion of aromatic proton signals
When the spectrum is examined carefully, the signals arising from impurities can be identified.

Acetaminophen purity 98.4% (qNMR method)
(RSD of three measurements = 0.1%)

Formula (1)

$$P_{\text{sample}} = \frac{I_{\text{sample}}}{I_{\text{std}}} \times \frac{H_{\text{sample}}}{H_{\text{std}}} \times \frac{m_{\text{sample}}}{m_{\text{std}}} \times \frac{M_{\text{sample}}}{M_{\text{std}}} \times P_{\text{std}}$$

- I = signal intensity (integration value)
- H = proton number (number of protons in the functional group)
- m = mass (basis weight value)
- M = molecular weight
- p = purity (%)



Purity analysis by NMR is important to improve the reliability of quantitative analysis.*3

When the purity of a standard material to be used for quantitative analysis, such as a chromatographic method, is not certain, it is still possible to determine the purity using qNMR.

Improving the known purity of standard substances therefore improves the reliability of quantitative analysis that can be obtained by chromatographic or similar methods.

*1 The JEOL method for internal standard quantitation (qNMR) is "AQARI" (Accurate Quantitative NMR with Internal reference substance) and supports comprehensive analytical operation from sample preparation to analysis.

*2 1,4-BTMSB- d_4 standard product regulation Trace Sure: Code No. 024-17031 Wako Pure Chemical Industries, Ltd.

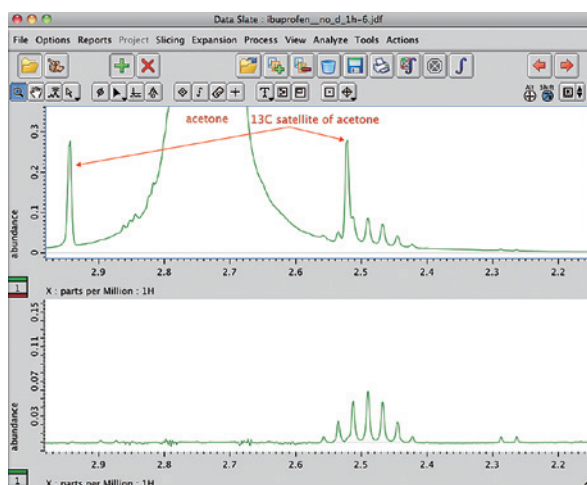
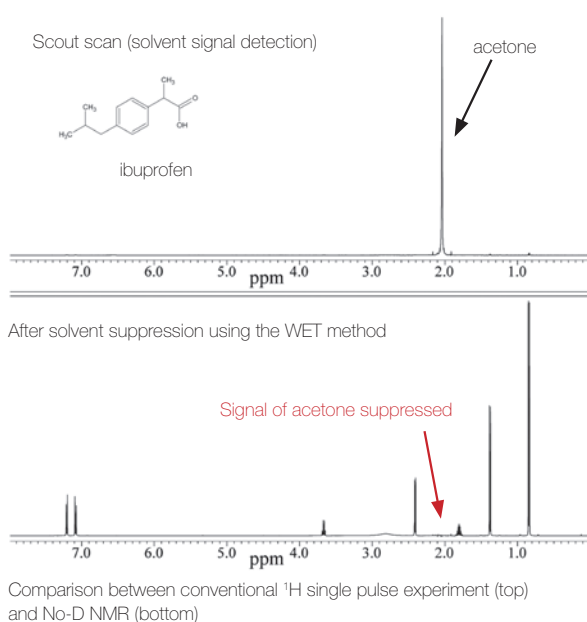
*3 Toshihide Ihara, Takeshi Saito, JEOL NEWS, 44, 1-10 (2012) "Realization of innovative calculation traceability by quantitative NMR"

No-D NMR

Low cost, high throughput

“No-D NMR” is a method to measure NMR spectra in low cost, non-deuterated solvents, e.g. when a sample is isolated by chromatography. As the process of solvent substitution is eliminated, it can greatly shorten the required time from isolation to NMR measurement.

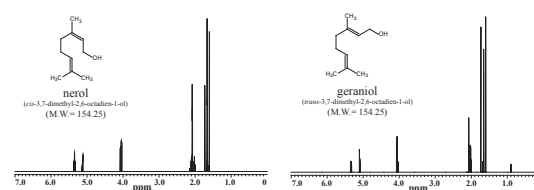
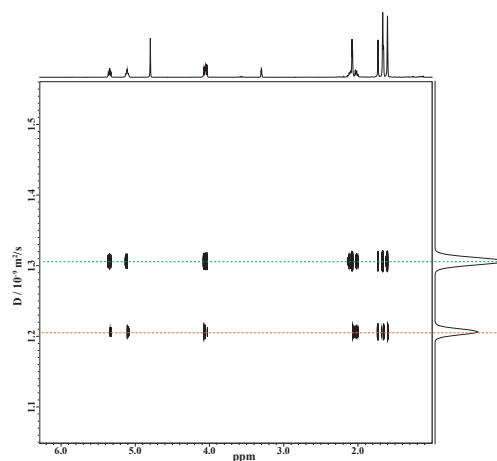
“No-D NMR” incorporates measurement with no NMR lock as an automatic function. The spectrometer is capable of automatic selective shimming on ^1H , detecting and suppressing the solvent resonance, and properly referencing the resulting spectra. This allows for routine “No-D NMR” experiments.



DOSY (Diffusion Ordered Spectroscopy)

Mixture using self diffusion coefficient

The DOSY method is mainly used for the analysis of mixtures. Signals arising from each component within a mixed sample are separated by their different self diffusion coefficients. It can analyze additives and impurities, reaction intermediates which may not be possible to isolate, polymerization of monomers, etc. without affecting the chemical or physical condition of the sample. The high performance of the JNM-ECZS spectrometer and various algorithms standard within Delta software allow for separation which was assumed to be difficult in the past.

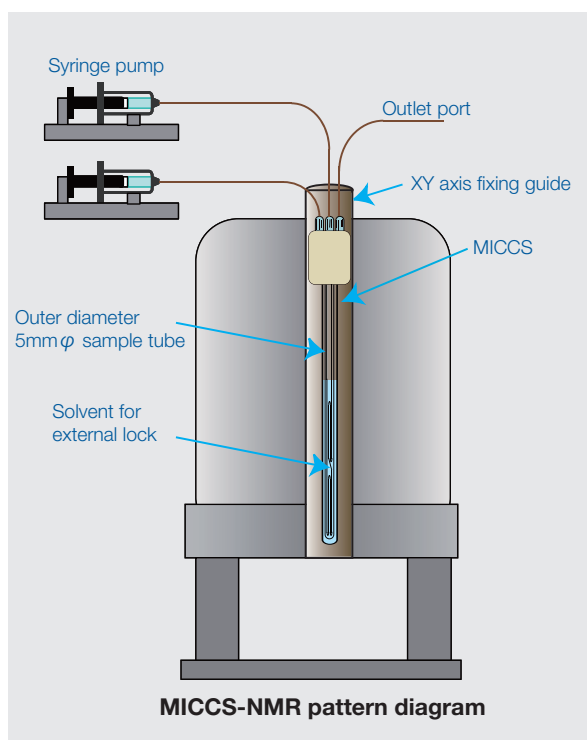
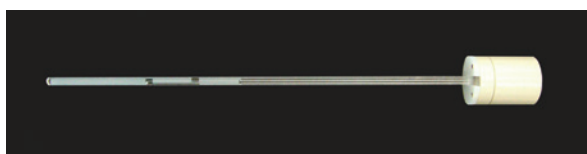


Slices of nerol (left) and geraniol (right) extracted from the DOSY spectrum

MICCS

Real time monitoring of chemical reactions

MICCS (Micro Channeled Cell for Synthesis monitoring) is an interface microcell for NMR, designed to be used with standard JEOL NMR probes. In MICCS-NMR, reagent solutions are introduced from 2 or 3 different ports on top of the cell using syringe pumps, and thus reaction occurs within the MICCS cell in the NMR probe. Thus MICCS enables real time monitoring of chemical reactions by NMR.



MICCS-NMR

Multivariate Analysis

Analysis of multi-component mixtures using statistical processing

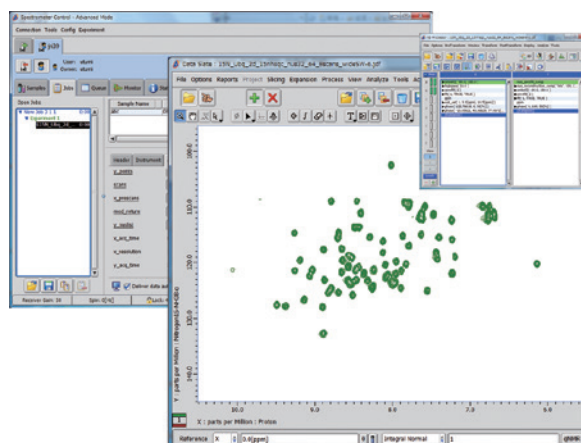
The JNM-ECZS spectrometer is also suitable for metabolomics. One can use the proton spectrum of a metabolite to obtain knowledge on a clinical condition by conducting pattern recognition and classification between samples through multivariate analysis. JNM-ECZS can automatically execute the various measurements needed for metabolomic analysis such as solvent suppression, T_2 and diffusion filters, and obtaining J -resolved spectra. As multivariate analysis is applicable to various samples, instead of being limited to metabolites only, a wider range of applications are possible.

“ALICE2 for Metabolome” (option) is a fully automated software that covers multi-sample processing to statistical analysis of the data. This software has been developed through joint research with the Medical Magnetic Resonance Analysis Facility, Nippon Medical School (Head: Dr. Yokichi Ohno).

NUS (Non Uniform Sampling)

Great reduction of measurement time for multi-dimensional data

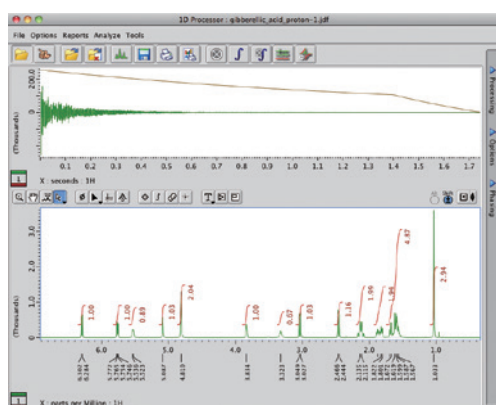
Non Uniform Sampling makes measurements faster by nonlinearly omitting acquisition of some data points in the indirect observation axis of multi-dimensional NMR. This method can yield spectra which are equivalent to conventionally acquired data by reconstructing the omitted data using a mathematical algorithm. Even with the smaller number of data points actually measured, data can be obtained without degradation of digital resolution. As measurement time is proportional to the number of data points on the indirect observation axis, this method can greatly reduce measurement time.



Powerful NMR data processing software

Delta

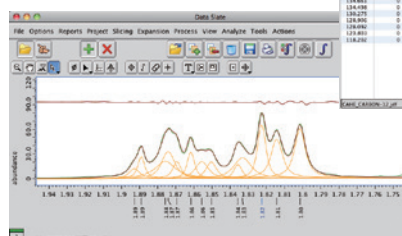
Delta is a powerful and fully integrated software platform for NMR measurement and data processing. Equipped with all functions necessary for general and advanced data processing and analysis of NMR data, it continues to advance as the best NMR software with innovative multiple functionality and user friendliness. The interface and pop-up helps are available in several languages, including English, Chinese and Russian.



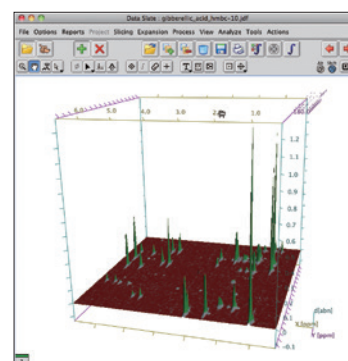
1D processor



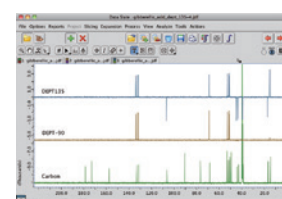
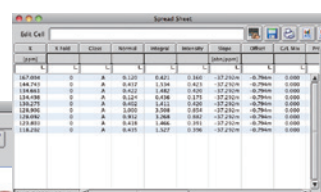
Pop up help



Waveform separation



3D display

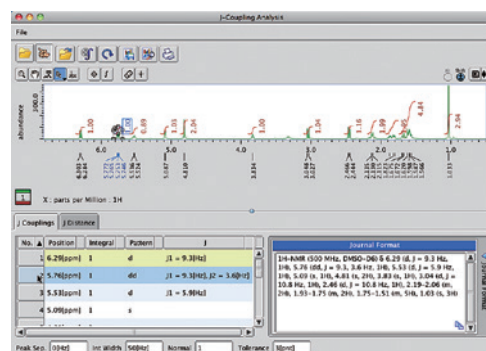


Overlay display

Assistance for report creation

The *J*-coupling analysis tool can analyze splitting patterns and determine *J*-coupling constants immediately once peak picking and peak integrals are loaded.

The result can be edited by the user within the tool, and the generated text can be copied to clipboard or saved in a text format.

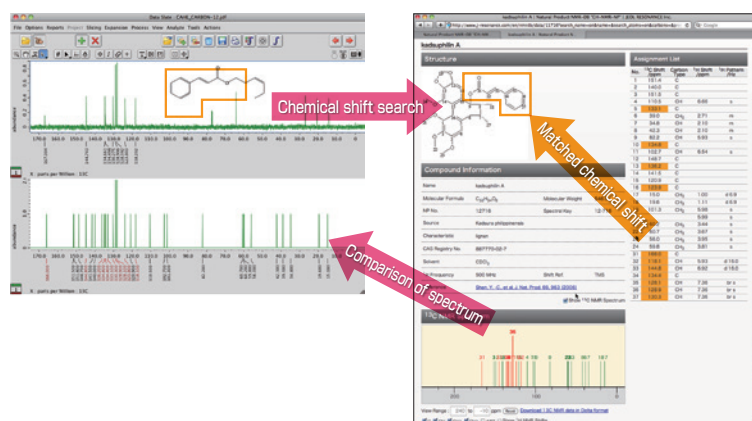


J coupling analysis tool

Linked to the natural organic compound NMR database “CH-NMR-NP”

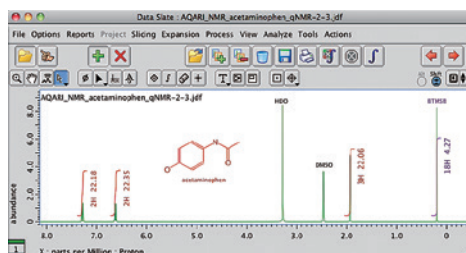
Delta also has a function that allows for easy linkage with the natural organic compound NMR database “CH-NMR-NP” by Dr. Kikuko Hayamizu. With Delta, a direct comparison between the search result from CH-NMR-NP and the spectrum is possible. Also, using data in Delta format, manual input of chemical shifts is not needed.

* CH-NMR-NP is an NMR database of natural organic compounds, and is available free of charge at the JEOL web site (<http://www.jeol.co.jp/en>).



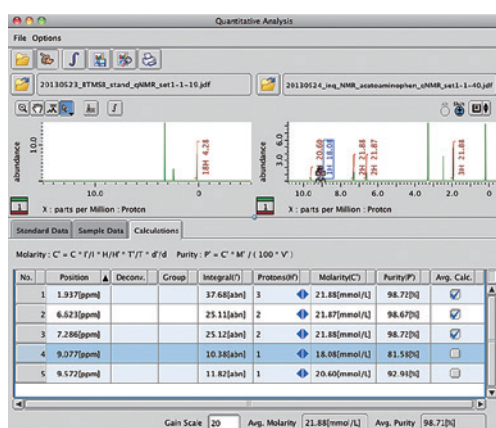
Various NMR quantification methods

Delta is equipped with the qNMR module. (See p.8) Once the number of protons for each signal is defined, the concentration ratio of each component is automatically calculated instead of displaying the more general integration value.



Spectrum of qNMR mode

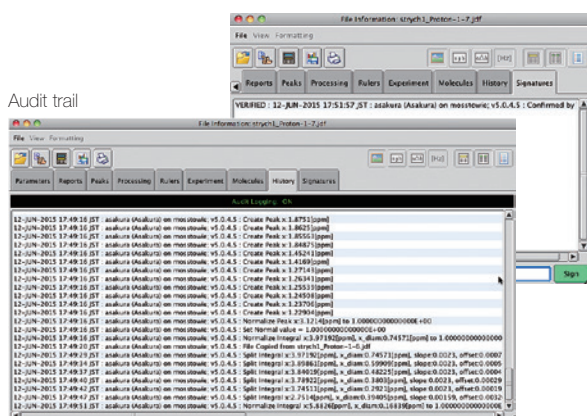
The quantitative analysis tool supplied with Delta can easily calculate concentration and purity, not only by AQARI (See p.8, internal standard reference), but also using a simple external standard reference such as PULCON.



Quantitative analysis tool

Audit trail and electronic signature

Delta is equipped with functions necessary for electronic recording and electronic signature compliant with ER/ES guidelines of the Ministry of Health, Labour and Welfare, ANNEX 11 of European Union (EU), and 21 CFR Part11 of the FDA in USA.



Audit trail

Free download

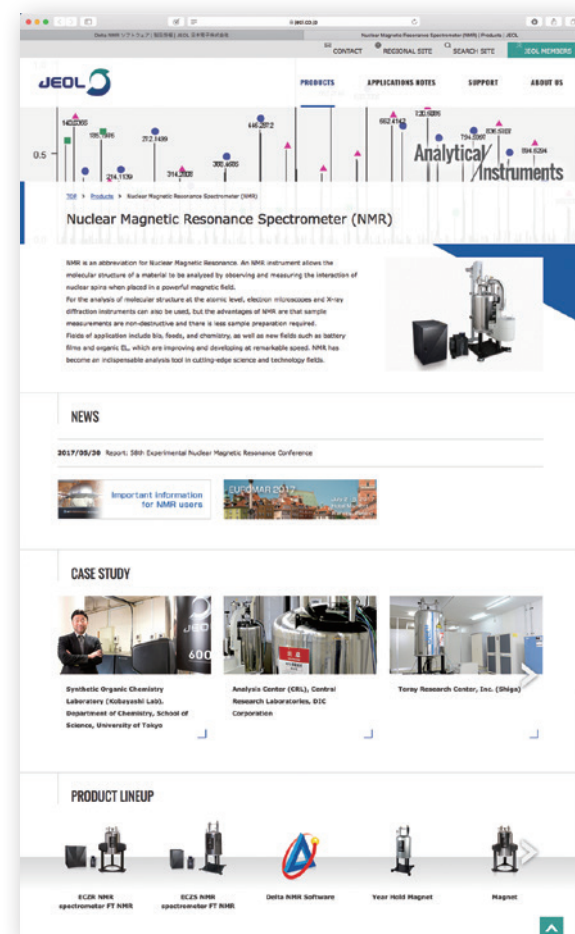
Delta, the standard data processing software of ECZ series, is free to download from the JEOL web site (www.jeol.co.jp/en/) *1.

Available for both Windows® and Mac OS X, it is exactly the same software as that supplied with an instrument, and most data processing functions can be performed on your PC *2. A user's manual is included and tutorial movies are also available on the web site. As Delta supports various non-JEOL data formats, you can enjoy the analysis of NMR data at your own desk *3.

*1 Free user registration on the web site is required for continuous operation. Also, free software is offered without support.

*2 Depending upon the many different environments where MS-Windows® or Mac OS X is installed, there is still a possibility that Delta does not work properly depending on the configuration and performance of the PC used.

*3 For non-JEOL data, Delta software will apply basic FID data processing. Also, in data formats other than JEOL format, some special operations may be needed in processing the data.



JEOL web site
<https://www.jeol.co.jp/en/products/detail/Delta5.html>

* Windows a registered trademark of Microsoft Corporation in USA and other countries.

* Mac OS X a registered trademark of Apple Inc in the United States and other countries

More reliable, safe, comfortable and economical NMR system

Proven anti-vibration mechanism did not fail during the Great Tohoku Earthquake on March 11, 2011.

The anti-vibration mechanism and base plate that JEOL uses for SCMs, are designed to reduce minor vibrations coming from the floor that adversely affect NMR spectra. However, this highly reliable anti-vibration mechanism is the only one used by NMR manufacturers to withstand the Great Tohoku Earthquake in 2011 and prevented damage to JEOL SCMs. JEOL's anti-vibration mechanism has also prevented damage to SCMs in previous earthquakes.

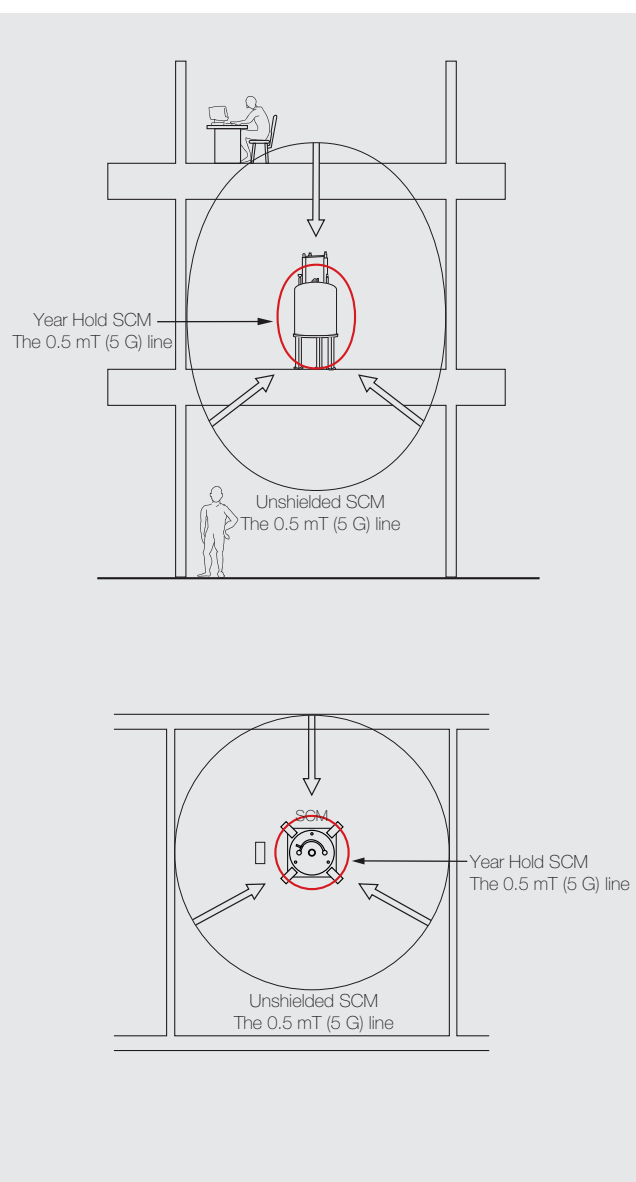
By combining a low point of gravity from the base plate held by anchor bolts, when disaster strikes, the risk of damage can be reduced to the minimum.

Guaranteed drift rate 4 Hz/hr or lower

In general, the magnetic field stability required for high resolution NMR systems is 5 Hz/hr or less. JEOL guarantees a magnetic field drift rate of 4 Hz/hr or less for stability which is a pre-requisite for high quality spectra. JEOL's SCM affords all the performance necessary for obtaining high resolution spectra and can be used confidently by anyone with minimal training.

Self-shielded SCM

JEOL's new 400 MHz Year Hold SCM (400JJYH) greatly improves the hold time of liquid helium while maintaining its compact size. "400JJYH" magnet reduces the helium filling period to once a year with the cryostat kept compact. A newly-designed superconducting coil reduces leakage of magnetic fields from inside to outside. Combined with a compact spectrometer console of the JNM-ECZS, the layout of installation area is made more flexible, enabling all units to be placed in a narrower area. The magnetic shield of SCM reduces not only the field leakage but also external influences. Thus, several NMR systems can be placed close to each other, allowing NMR systems to be used more reliably, safely, comfortably and economically.



No need for routine refilling of liquid nitrogen!

The nitrogen recycler "NR-50" (option) re-liquefies the nitrogen gas evaporated from the SCM, and returns it to the SCM. Hence the weekly liquid nitrogen refill is no longer needed.

The NR-50 employs a compact air-cooled cryogenic freezer that works from a single phase power supply and does not need cooling water, leading to both low investment cost and low running cost.



Year-hold magnet reduces liquid helium consumption

The 400JJYH is a compact low-consumption magnet that uses innovative super conducting materials and an extremely low helium evaporation rate. It is almost the same size as 400JJ magnet.

The helium consumption is reduced by 39% when compared with previous year-hold magnets *1.

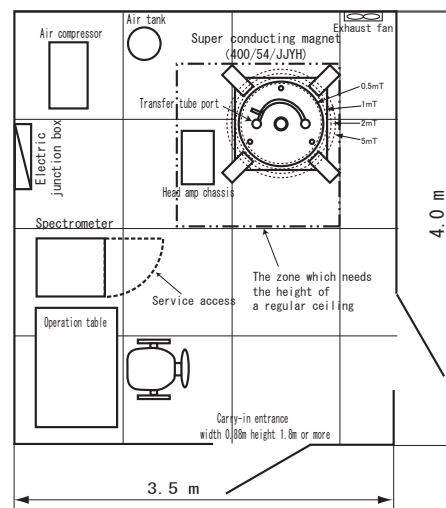


*1 Liquid helium refill volumes:
400JJYH 120 L, 400/54SSYHWS 195 L

Installation Requirement

Required power supplies (breaker) and grounding

Spectrometer	Single phase AC100 V to 240 V, 50/60 Hz, 1.5 kVA
Data system	Single phase AC100 V to 240 V, 50/60 Hz, 1 kVA
Air compressor (400 MHz)	Single phase AC100 V, 50/60Hz, 3 kVA



Installation example of 400 MHz



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